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High-resolution photoemission spectroscopy on intermediate valent Yb-compounds: predictions of the Anderson impurity model

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Abstract

We have analyzed high-resolution photoemission spectroscopy data on the 4f spectral function of various intermediate valent Yb-systems. The photoemission results are internally consistent with the predictions of the single-impurity Anderson model, but reveal quantitative discrepancies compared to the results from bulk-sensitive measurements.

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For the understanding of strongly correlated rare-earth systems the simplest theoretical description is the single-impurity Anderson model (SIAM). While the model is successful in describing the thermodynamic and magnetic properties of solids, problems have been reported in the application to photoemission results on rare-earth compounds. To investigate these discrepancies, we have performed high-resolution photoemission spectroscopy (PES) on a series of intermediate valent (IV) ytterbium compounds with valencies $v_{Yb} = 2.40$–2.91 ($\Delta E \approx 6$ meV). From the spectra we have extracted the binding energy ε_0 of the Yb $4f^{13}_{7/2}$ peak (sometimes identified as the Kondo resonance) close to the Fermi energy as well as the hole occupation number n_h ($v_{Yb} = 2 + n_h$) which is determined from the distribution of the 4f spectral weight at low temperatures ($T \approx 20$ K). Fig. 1c clearly shows the monotonous dependence of the n_h-values from ε_0. According to the SIAM, $n_h(\varepsilon_0)$ should be approximately given by $n_h(\varepsilon_0) = \Delta/(\Delta + \varepsilon_0)$. The dashed line in Fig. 1c shows that the two PES parameters can be correlated consistently by using a constant Δ. The next step is to investigate how the PES-parameters are related to the thermodynamic properties described by, e.g., T_{max} (maximum of $\chi(T)$, see inset Fig. 1b) and χ_0^{-1} as shown in Fig. 1b and a. Obviously, there is also a monotonous dependence. Since ε_0 describes the low-energy scale in PES, we relate ε_0 from PES to the characteristic energy scale $k_B T_0$ (characteristic temperature T_0) from thermodynamic measurements and set $\varepsilon_0 = n_h k_B T_0$ with $T_0 = \alpha^{-1} T_{max}$. However, while we obtain a good qualitative fit of $\chi_0(\varepsilon_0)$ and $T_{max}(\varepsilon_0)$ from the relation $\chi_0 = (\mu_{eff}^2 n_h)/(3k_B T_0)$ [1] in Fig. 1b and a, the resulting value α from the fit is by a factor of ~ 2 too small in comparison to the value predicted by the SIAM [2]. The reason for this quantitative deviation might be that the SIAM is too simple in its principle because it neglects, e.g., lattice

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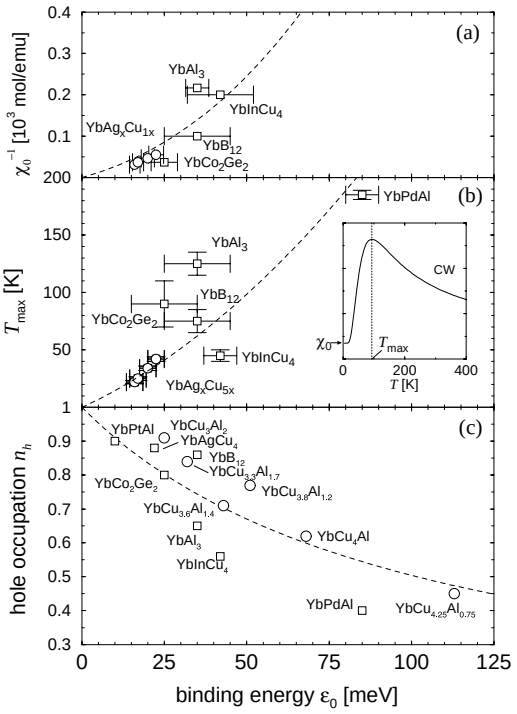

Fig. 1. Consistency of PES results and comparison to magnetic susceptibility measurements. Fig. c shows the $n_h(\varepsilon_0)$ dependence of the UPS data and the fit according to the SIAM (dashed line). (a) and (b) display the results from magnetic susceptibility measurements (low-temp. susceptibility χ_0 and characteristic temperature T_0, see inset). The fits use the same parameter $\Delta = 103$ meV from c.

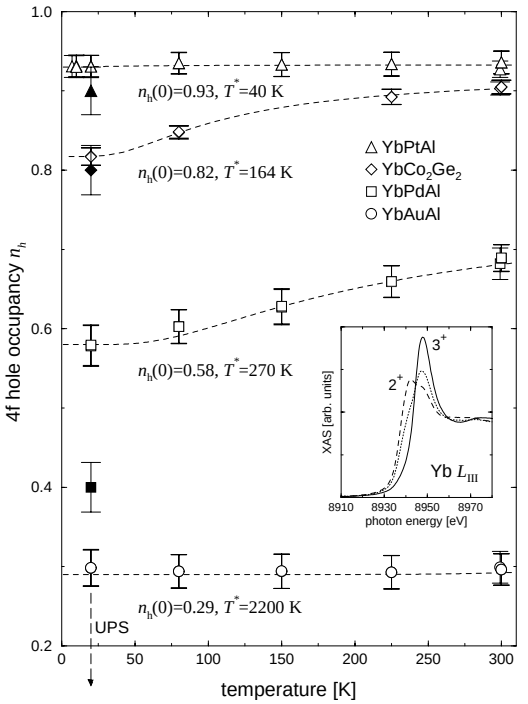

Fig. 2. Temperature dependence of n_h from Yb L_{III} XAS data (inset: the XAS data is analyzed by decomposition of the L_{III}-edge into the 2^+- and 3^+-contribution to extract n_h [3]). The dashed lines: fit according to the SIAM. The filled symbols denote the low-temperature $n_h(T)$-value from UPS, see Fig. 1c.

effects. On the other hand, PES is highly surface-sensitive in comparison to thermodynamic and magnetic measurements. Therefore, we have used X-ray absorption spectroscopy (XAS) as an additional spectroscopic method with negligible surface contributions. In Fig. 2 we show the XAS $n_h(T)$-curves for the compounds YbPtAl, $YbCo_2Ge_2$, YbPdAl and YbAuAl. In comparison to the low-temperature UPS results for n_h, the XAS values are systematically larger. From this point of view the results from XAS confirm the quantitative deviations of the PES results from those from bulk sensitive thermodynamic and magnetic measurements. Since all experimental methods seem to be described well within the SIAM but require different values for the model parameters in the case of PES, this could be a hint that the observed deviations may be caused by surface effects.

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